

# Modular networks emerge from multiconstraint optimization

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Modular structure is ubiquitous among complex networks. We note that most such systems are subject to multiple structural and functional constraints, e.g., minimizing the average path length and the total number of links, while maximizing robustness against perturbations in node activity. We show that the optimal networks satisfying these three constraints are characterized by the existence of multiple subnetworks (modules) sparsely connected to each other. In addition, these modules have distinct hubs resulting in an overall heterogeneous degree distribution.

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Complex networks have recently become a focus of scientific attention, with many natural, social and technological networks seen to share certain universal structural features [1, 2]. These networks often exhibit topological characteristics that are far from random. For instance, they show a significant presence of *hubs*, i.e., nodes with large degree or number of connections to other nodes. Indeed, hubs are crucial for linking the nodes in real networks, which have extremely sparse connectivity, with the probability of connection between any pair of nodes,  $C$ , varying between  $10^{-1}$  and  $10^{-8}$  [1]. By contrast, random networks with such small  $C$  are almost always disconnected. The hubs also lead to the “small-world” effect [3] by reducing the average path length of the network. Another property observed in many networks is the existence of a modular structure. We define a network to be *modular* if it exhibits significantly more intramodular connections compared to intermodular connections. Such networks can be decomposed into distinct subnetworks or modules by removing a few links. Modular networks observed in empirical studies span a wide range from cellular networks involved in metabolism and signalling [4], to cortical networks [5], social networks [6], food webs [7] and the internet [8]. Many of these networks also exhibit large number of hubs, which often have the role of interconnecting different modules [9].

The majority of previous studies on modular networks have been concerned with methods to identify community structure [10]. There have been relatively few attempts to explain the potentially more interesting question of how and why modularity emerges in complex networks. Most such attempts are based on the notion of evolutionary pressure, where a system is driven by the need for adapting to a changing environment [11, 12]. However, such explanations involve complicated adaptive mechanisms, in which the environment itself is assumed to change in a modular fashion. Further, adaptation might lead to decrease in connectivity through biased selection of sparse networks, which eventually results in *disruption of the network* with the modules being isolated nodes [11] or disconnected parts [13]. More recently, a social network model has shown the emergence of isolated communities through the rearrangement of links to form groups with homogeneous opinion [14].

A crucial limitation of these above studies is that they almost always focus on a single performance parameter. However, in reality, most networks have to optimize between several, often conflicting, constraints. While structural constraints, such as path length, had been the focus of initial work by network researchers, there has been a growing realization that most networks have dynamics associated with their nodes [15]. The robustness of network behavior is often vital to the efficient functioning of many systems, and also imposes an important constraint on networks. Therefore, the role played by dynamical considerations in determining the topological properties of a network is a challenging and important question that opens up new possibilities for explaining observed features of complex networks [16]. In this letter, we propose a simple mechanism for the emergence of modularity in networks as an optimal solution for satisfying a minimal set of structural and functional constraints. These essentially involve (i) reducing the average path length,  $\ell$ , of a network by (ii) using a minimum number of total links,  $L$ , while (iii) decreasing the instability of dynamical states associated with the network.

We investigate the dynamical stability of a network composed of  $N$  nodes, which are self regulating when isolated, by measuring the growth rate of a *small* perturbation  $\mathbf{x}$  about an equilibrium state of the network dynamics. Although the system can be nonlinear in general, the dynamics of such perturbations are described by a *linear* system of coupled differential equations  $\dot{x}_i = \sum_{j=1}^N J_{ij} x_j$ . The stability of the equilibrium is then determined by the largest real part  $\lambda_{\max}$  of the eigenvalues for the matrix  $\mathbf{J}$  representing the interactions among the nodes. The perturbation decays if  $\lambda_{\max} < 0$ , and increases otherwise, at a rate proportional to  $|\lambda_{\max}|$ . Thus, minimizing  $\lambda_{\max}$  makes the equilibrium less unstable, which is important for many systems including ecological networks [17]. Here  $J_{ii} = -1 \forall i$  such that we only consider instability induced through network interactions. The off-diagonal matrix elements  $J_{ij} (\sim A_{ij} W_{ij})$  include information about both the topological structure of the network, given by the adjacency matrix  $\mathbf{A}$  ( $A_{ij}$  is 1, if nodes  $i, j$  are connected, and 0, otherwise;  $A_{ii} = 0 \forall i$ ), as well as, the distribution of interaction strengths  $W_{ij}$  between nodes. In our simulations,  $W_{ij}$  has a Gaussian

distribution with zero mean and variance  $\sigma^2$ ; however, a nonzero mean does not qualitatively change our results. For an Erdős-Rényi (ER) random network,  $\mathbf{J}$  is a sparse random matrix, with  $\lambda_{\max} \sim \sqrt{NC\sigma^2} - 1$ , according to the May-Wigner theorem [17]. Therefore, increasing the system size  $N$ , connectivity  $C$  or interaction strength  $\sigma$ , results in instability of the network. This result has been shown to be remarkably robust with respect to various generalizations [18]. Further, for uniform coupling strength,  $\lambda_{\max}$  is inversely related to the epidemic propagation threshold for the network [19], and hence, minimizing  $\lambda_{\max}$  also makes the network more robust against spreading of infection.

Networks are also subject to certain structural constraints. One of them is the need to save resources, manifested in minimizing *link cost*, i.e., the cost involved in building and maintaining each link in a network [20]. This results in the network having a small total number of links,  $L$ . However, such a procedure runs counter to another important consideration of reducing the average path length  $\ell$ , which improves the network *efficiency* by increasing communication speed among the nodes [21]. The conflict between these two criteria can be illustrated through the example of airline transportation networks. Although, fastest communication (i.e., small  $\ell$ ) will be achieved if every airport is connected to every other through direct flights, such a system is prohibitively expensive as every route involves some cost in maintaining it. In reality, therefore, one observes the existence of airline hubs, which act as transit points for passengers arriving from and going to other airports.

For ER random networks, although  $\ell$  is low,  $L$  is high because of the requirement to ensure that the network is connected:  $L > N \ln N$  [22]. Introducing the constraint of link cost (i.e., minimizing  $L$ ) while requiring low average path length  $\ell$ , leads to a starlike connection topology (Fig. 1C). A *star network* has a single hub to which all other nodes are connected, there being no other links. Its average degree  $\langle k \rangle \approx 2$  is *non extensive* with system size, and is much smaller than a connected random network, where  $\langle k \rangle \sim \ln N$ . However, such starlike networks are extremely unstable with respect to dynamical perturbations in the activity of their nodes. The probability of dynamical instability in random networks increases only with average degree ( $\lambda_{\max} \sim \sqrt{\langle k \rangle}$ , since  $\langle k \rangle = NC$ ), while for star networks it increases with the largest degree, and hence the size of the network itself ( $\lambda_{\max} \sim \sqrt{N}$ ). To extend this for the case of weighted networks we look at the largest eigenvalue of  $\mathbf{J}$ ,  $\lambda_{\max} = -1 + \sqrt{\sum_{i=2}^N J_{1i} J_{i1}}$ , the hub being labeled as node 1. The stability of the weighted star network is governed by  $\sum_{i=2}^N J_{1i} J_{i1}$ , which is the displacement due to a 1-dimensional random walk of  $N - 1$  steps whose lengths are products of pairs of random numbers chosen from a *Normal* ( $0, \sigma^2$ ) distribution.

To obtain networks which satisfy the dynamical as well as the structural constraints we perform optimization us-

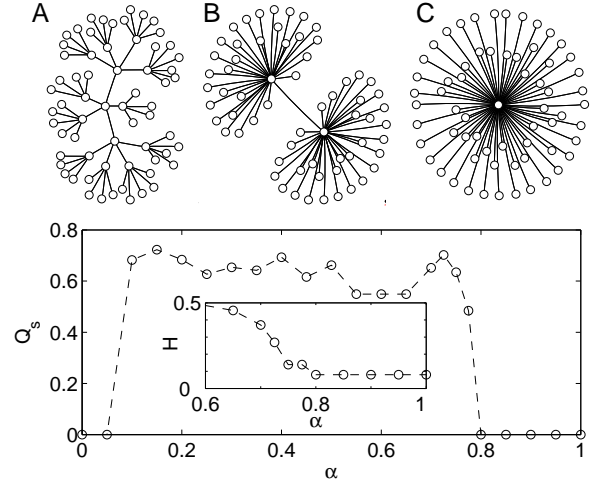


FIG. 1: The optimized network structures for a system with  $N = 64$  nodes and  $L = N - 1$ , at different values of  $\alpha$ : (A) 0.4, (B) 0.775 and (C) 1. For  $\alpha = 0$  the optimal network is a 1-dim chain. (Bottom) The modularity  $Q_s$  of the optimized network for different  $\alpha$ , when each module is a community defined in the strong sense. The transition to star configuration occurs around  $\alpha \simeq 0.8$ , as observed in the variation of degree entropy  $H$  with  $\alpha$ .

ing simulated annealing, with a network having  $N$  nodes and  $N - 1$  unweighted links (the smallest number that keeps the network connected). Having fixed  $L$ , the energy function to be minimized is defined as

$$E(\alpha) = \alpha \ell + (1 - \alpha) \lambda_{\max},$$

where the parameter  $\alpha \in [0, 1]$  denotes the relative importance of the path length constraint over the condition for reducing dynamical instability. Rewiring is attempted at each step and is (i) rejected if the updated network is disconnected, (ii) accepted if  $\delta E = E_{\text{final}} - E_{\text{initial}} < 0$ , and (iii) if  $\delta E > 0$ , then accepted with probability  $p = \exp(-\delta E/T)$ , where  $T$  is the “temperature”. The initial temperature was chosen in such a way that energetically unfavorable moves had 80% chance of being accepted. After each monte carlo step ( $N$  updates) the temperature was reduced by 1% and iterated till there was no change in the energy for 20 successive monte carlo steps. For each value of  $\alpha$ , the optimized network with lowest  $E$  was obtained from 100 realizations.

As can be seen from Fig. 1, modularity emerges when the system tries to satisfy the twin constraints of minimizing  $\ell$  as well as  $\lambda_{\max}$ . When  $\alpha$  is very high ( $\sim 0.8$ ) such that the instability criterion becomes less important, the system shows a transition to a starlike configuration with a single hub. However, as  $\alpha$  is decreased, the instability of the hub makes the star network less preferable and for intermediate values of  $\alpha$ , the optimal network gets divided into modules, as seen from the measure of network modularity,  $Q$  [23]. This is defined as  $Q = \sum_s [(L_s/L) - (d_s/2L)^2]$ , where  $L_s$  is the number

of links between nodes within a module  $s$ , and  $d_s$  is the sum of the degrees of the nodes in  $s$ . To obtain a robust partitioning of the network, we consider modules to be communities defined in the *strong* sense, i.e., each node  $i$  belonging to a community has more connections with nodes within the community than with the rest of the network [24]. The resulting modularity measure  $Q_s$  is high for a modular network, whereas for homogeneous, as well as, for starlike networks,  $Q_s = 0$ . To determine the communities, we (1) compute the betweenness measure for all edges and remove the one with highest score: (2a) if it results in splitting the network (or subnetwork) into communities in the strong sense, then the resulting  $Q_s$  is computed; (2b) if not, we go back to step (1) and remove the edge with the next highest score. The process is carried out iteratively until all edges of the network have been considered. Note that, in step (2a), checking whether the splitting results in communities in the strong sense is considered with respect to the full network. We verified these results by also calculating  $Q_s$  with the network modules determined through stochastic extremal optimization [25]. The transition between modular and star structures is further emphasised in the behavior of the degree entropy,  $H = -\sum_k p_k \ln p_k$ , where  $p_k$  is the probability of a node having degree  $k$ . The emergence of a dominant hub at a critical value of  $\alpha$  is marked by  $H$  reducing to a low value.

To understand why modular networks emerge on simultaneous optimization of structural and functional constraints we look at the change in stability that occurs when a star network is split into  $m$  modules, the modules being connected through links between their hubs. The largest eigenvalue for the entire system of  $N$  nodes is the same as that for each isolated module,  $\lambda_{\max} \sim \sqrt{N/m}$ , as the additional effect of the few intermodular links is negligible. At the same time, the increase in the average path length  $\ell$  with  $m$  is almost insignificant. Therefore, by dividing the network into a connected set of small modules, each of which is a star subnetwork, the instability of the entire network decreases significantly while still satisfying the structural constraints.

The above results were obtained for a specific value of  $L$  ( $= N - 1$ ). We now relax the constraint on link cost and allow a larger number of links than that strictly necessary to keep the network connected. The larger  $L$  is manifested as random links between nonhub nodes, resulting in higher clustering within the network. Even for such *clustered star* networks,  $\lambda_{\max}$  increases with size as  $\sqrt{N}$ , and therefore, their instability is reduced by imposing a modular structure (Fig. 2). The effect of increasing the number of modules,  $m$ , on the dynamical stability of a network can be observed from the stability-instability transition that occurs on increasing the network parameter  $\sigma$  keeping  $N, C$  fixed. The critical value at which the transition to instability occurs,  $\sigma_c$ , increases with  $m$  (Fig. 2, inset) while  $\ell$  does not change significantly. This signifies that even for large  $L$ , networks satisfy the structural and functional constraints by adopting a modular

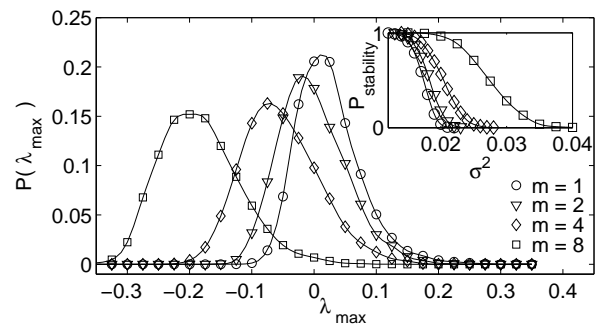


FIG. 2: Probability distribution of  $\lambda_{\max}$  for a clustered star network ( $N = 256, L = 15N$ ) with different numbers of modules,  $m$ . Modules of equal size are connected by single link between respective hubs. Link weights  $W_{ij}$  follow a *Normal* ( $0, \sigma^2$ ) distribution with  $\sigma^2 = 0.018$ . (Inset) Probability of stability [ $P(\lambda_{\max} < 0)$ ] varying with  $\sigma^2$ . Increasing  $m$  results in the transition to instability occurring at higher  $\sigma^2$ , implying that network stability increases with modularity.

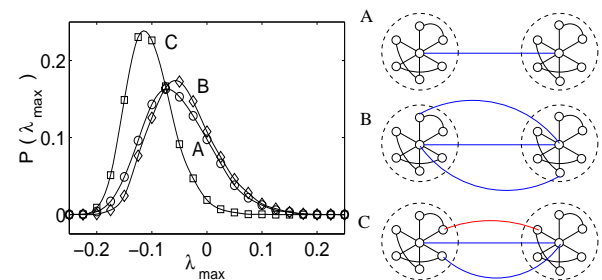


FIG. 3: Probability distribution of  $\lambda_{\max}$  for clustered star networks ( $N = 256, L = 15N$ ) having four modules with different types of intermodular connectivities (A), (B) and (C), which are represented schematically here. Link weights  $W_{ij}$  have a *Normal* ( $0, \sigma^2$ ) distribution with  $\sigma^2 = 0.018$ .

configuration.

As  $L$  is increased, we observe that the additional links in the optimized network occur between modules, in preference to, between nodes in the same module. To see why the network prefers the former configuration, we consider three different types of intermodular connections: (A) only the hub nodes of different modules are connected, (B) nonhub nodes of one module can connect to the hub of another module, and (C) nonhub nodes of *different* modules are connected. Arrangement (B) where intermodular connections that link to hubs of other modules actually increase the maximum degree in the modules, making this arrangement more unstable than (A). On the other hand, (C) connections between nonhub nodes of *different* modules not only decrease the instability (Fig. 3), but also reduce  $\ell$ . As a result, the optimal network will always prefer this arrangement (C) of large number of random intermodular connections over other topologies for large  $L$ .

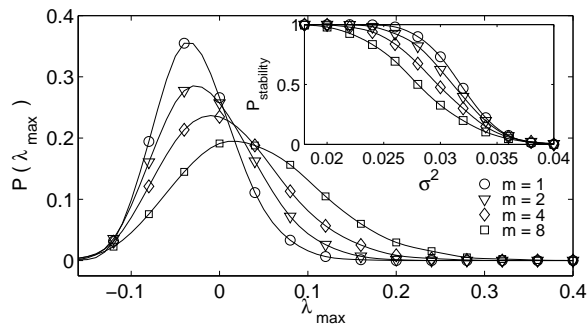


FIG. 4: Probability distribution of  $\lambda_{\max}$  for random networks ( $N = 256, L = 15N$ ) as a function of the number of modules,  $m$ , which are connected to each other by single links. Link weights  $W_{ij}$  follow  $Normal(0, \sigma^2)$  distribution with  $\sigma^2 = 0.03$ . The inset shows the probability of stability [ $P(\lambda_{\max} < 0)$ ] varying with  $\sigma^2$ . Increasing  $m$  results in transition to instability at lower  $\sigma^2$ , indicating that increasing modularity decreases stability for random networks.

Our observation that *both* structural and dynamical constraints are necessary for modularity to emerge runs counter to the general belief that modularity necessarily follows from the requirement of robustness *alone*, as modules are thought to limit the effects of local perturbations in a network. To further demonstrate that the three constraints are the minimal required for a network to adopt a modular configuration, we remove the hub from a clustered star while ensuring that the network is still connected. This corresponds to the absence of the link cost constraint altogether and the optimal graph is now essentially a random network. To see why modularity is no longer observed in this case, we consider the stability of an ER random network on which a modular structure has been imposed. A network of  $N$  nodes is divided into  $m$  modules, connected to each other with a few intermodular links. We then consider the stability-instability transition of networks for increasing  $m$ , with

the average degree,  $\langle k \rangle$  kept fixed. Although from the May-Wigner theorem, it may be naively expected that  $\sigma_c \simeq 1/\sqrt{\langle k \rangle}$  is constant w.r.t.  $m$ , we actually observe that increasing  $m$  decreases stability (Fig. 4). This is because when a network of size  $N$  is split into  $m$  modules, the stability of the entire network is decided by that of the most unstable module, ignoring the small additional effect of intermodular connections. Thus, the stability of the entire network is decided by randomly drawing  $m$  values from the distribution of  $\lambda_{\max}$  for the modules. Therefore, for modular networks it is more likely that a positive  $\lambda_{\max}$  will occur, than for the case of a homogeneous random network of size  $N$  [26]. The *decrease* of stability with modularity for random networks shows that, in general, it is not necessary that modularity is always stabilizing and results in a robust network, as has sometimes been claimed [11].

In this paper we have shown that modules of interconnected nodes can arise as a result of optimizing between multiple structural and functional constraints. In particular, we show that by minimizing link cost as well as path length, while at the same time increasing robustness to dynamical perturbations, a network will evolve to a configuration having multiple modules characterized by hubs, that are connected to each other. At the limit of extremely small  $L$  this results in networks with bimodal degree distribution, that has been previously shown to be robust with respect to both targeted and random removal of nodes [27]. Therefore, not only are such modular networks dynamically less unstable, but they are also robust with respect to structural perturbations. In general, on allowing larger  $L$ , the optimized networks show heterogeneous degree distribution that has been observed in a large class of networks occurring in the natural and social world, including those termed as scale free networks [2]. Our results provide a glimpse into how the topological structure of complex networks can be related to functional and evolutionary considerations.

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